

# Application of hyperbolic scaling for calculation of reaction-subdiffusion front propagation

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A technique of hyperbolic scaling is applied to calculate a reaction front velocity in an irreversible autocatalytic conversion reaction  $A + B \rightarrow 2A$  under subdiffusion. The method, based on the geometric optics approach is a technically elegant observation of the propagation front failure obtained in Phys. Rev. E **78**, 011128 (2008).

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*Introduction.-* The problem of front propagation in reaction-transport equations is attracting much attention that is related to the considerable progress in our understanding of this phenomenon via the generalization of the standard reaction-diffusion scheme in the framework of the Fisher-Kolmogorov-Petrovskii-Piskunov (FKPP) equation for fractional reaction-subdiffusion systems [1–11]. The description of reactions under subdiffusion is relevant to strongly inhomogeneous environments, in porous media such as certain geological formations or gels, in crowded cell interiors, and so on. Another success in this field relates to developing an appropriate new technique of treating front propagation, where an appropriate hyperbolic scaling of the reaction-transport equation makes it possible to estimate the overall rate of the spreading reaction wave without resolving its shape [12, 13]. The method of hyperbolic scaling is based on the introduction of a small parameter  $\varepsilon \rightarrow 0$ , and rescaling of coordinates and time  $(x, t) \rightarrow (x/\varepsilon, t/\varepsilon)$ , and the contaminant's density distribution function. In this case, the problem of the wave propagation reduces to the dynamics of the leading edge, or the reaction front. Therefore, one analyzes the reaction-transport behavior in the leading edge, where, in the long-range and long-time limits, the detailed shape of the travelling wave is not important.

In this Report we demonstrate the hyperbolic scaling technique to calculate the reaction front velocity in an irreversible autocatalytic conversion reaction  $A + B \rightarrow 2A$  under subdiffusion, which, in the case of normal diffusion, is described by the FKPP equation [14, 15]. The present result is an alternative Hamilton-Jacobi approach via hyperbolic scaling, which is a more elegant presentation of the propagation front failure observed in Ref. [5].

Recent results show that, contrary to normal diffusion, the minimal propagation velocity is zero [5, 7, 8], which was interpreted as propagation failure (a general discussion of this issue can be found in [9]). The main focus was on situations when subdiffusion can be modelled within a continuous-time random walk (CTRW) scheme with a waiting-time probability density function (pdf) decaying according to the power law,  $\psi(t) \sim t^\alpha$ , with  $0 < \alpha < 1$ . Analytical and numerical calculations [5, 10] corroborated this picture, and in the regime of small re-

action rates, for which the continuous description applies, the front velocity was observed to go as  $t^{\frac{\alpha-1}{2}}$ . Crossover arguments, presented in [11], also support this picture.

*Reaction-transport equation.-* The FKPP equation describes a front propagating into the unstable state in bimolecular autocatalytic conversion  $A + B \rightarrow 2A$ . Initially, the whole system consists of particles of type  $B$ . The introduction of the  $A$ -individuals into some bounded spatial domain leads to the propagation of a front of  $A$  into the  $B$ -domain. A general reaction-transport scheme that corresponds to the irreversible  $A + B \rightarrow 2A$  reaction process can be described by the following generalization of the FKPP equation [1–6, 16, 17]

$$\begin{aligned} \frac{\partial B(x, t)}{\partial t} &= \frac{a^2}{2} \int_0^t \Delta \{M(t - t') B(x, t') \\ &\times \exp \left[ -k \int_{t'}^t [1 - B(x, t'')] dt'' \right] \} dt' \\ &- k[1 - B(x, t)] B(x, t). \end{aligned} \quad (1)$$

Here  $B(x, t)$  is a concentration of particles  $B$  with the initial condition  $B(x, t = 0) = B_0 = 1$ , and the condition of the mass conservation is

$$A(x, t) = 1 - B(x, t).$$

The time kernel  $M(\tau)$  is determined by the waiting time pdf in the Laplace domain  $\tilde{\psi}(u) = \hat{\mathcal{L}}[\psi(t)]$

$$\tilde{M}(u) = \frac{u \tilde{\psi}(u)}{1 - \tilde{\psi}(u)}. \quad (2)$$

*Hyperbolic scaling.-* In the sequel, we are concerned with the front propagation of particles/individuals of the type  $A$ . As mentioned above, to analyze the behavior of the leading edge, we use the technique of hyperbolic scaling developed in [12], see also [13], where the basic idea is that, in the long-range and long-time limit, the detailed shape of the travelling wave is not important, and the problem of wave propagation corresponds to the dynamics of the leading edge or the reaction front. We follow the details of the analysis presented in Refs. [17, 19]. It is convenient to rewrite Eq. (1) using the variable change in the integration with the memory kernel  $M(t -$

$t') \rightarrow M(t')$ . Thus Eq. (1) for type  $A$  individuals reads

$$\begin{aligned} \frac{\partial A}{\partial t} &= \sigma^2 \int_0^t \Delta \left\{ M(t') (A(x, t - t') - 1) \right. \\ &\quad \times \exp \left[ -k \int_{t-t'}^t [A(x, t'')] dt'' \right] \Big\} dt' \\ &\quad + k[1 - A(x, t)] A(x, t). \end{aligned} \quad (3)$$

After simple manipulation with the second derivative over space, it reads

$$\begin{aligned} \frac{\partial A}{\partial t} &= \sigma^2 \int_0^t M(t') \left\{ \Delta A(x, t - t') - k \nabla A(x, t - t') \right. \\ &\quad \times \int_0^{t'} \nabla A(x, t - t'') dt'' - k(A(x, t - t') - 1) \\ &\quad \times \int_0^{t'} \Delta A(x, t - t'') dt'' + k^2(A(x, t - t') - 1) \\ &\quad \times \left[ \int_0^{t'} \nabla A(x, t - t'') dt'' \right]^2 \Big\} \\ &\quad \times \exp \left[ -k \int_0^{t'} [A(x, t - t'')] dt'' \right] dt' \\ &\quad + k[1 - A(x, t)] A(x, t), \end{aligned} \quad (4)$$

where  $\sigma^2 = a^2/2$  and we use the  $t'' \rightarrow t - t''$ . The objective here is to find the rate of the front propagation  $v$  without resolving the shape of the travelling waves. We use hyperbolic scaling for the coordinates  $x$  and time  $t$

$$x \rightarrow \frac{x}{\varepsilon}, \quad t \rightarrow \frac{t}{\varepsilon},$$

and the rescaled density

$$A^\varepsilon(x, t) = A\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\right).$$

We write the density  $A^\varepsilon(x, t)$  in the exponential form

$$A^\varepsilon(x, t) = A_0 \exp \left[ -\frac{G^\varepsilon(x, t)}{\varepsilon} \right], \quad (5)$$

where the non-negative function  $G^\varepsilon(x, t)$  describes the asymptotics of the density function and plays a very important role in the theory of front propagation.

At the next step, we rescale  $x$  and  $t$  variables in Eq. (4) to obtain

$$\begin{aligned} \varepsilon \frac{\partial A^\varepsilon}{\partial t} &= \sigma^2 \int_0^{t/\varepsilon} M(t') \left\{ \Delta A^\varepsilon(x, t - t') \right. \\ &\quad - k \nabla A^\varepsilon(x, t - t') \int_0^{t'} \nabla A^\varepsilon(x, t - t'') dt'' \\ &\quad - k(A^\varepsilon(x, t - t') - 1) \int_0^{t'} \Delta A^\varepsilon(x, t - t'') dt'' \\ &\quad + k^2(A^\varepsilon(x, t - t') - 1) \left[ \int_0^{t'} \nabla A^\varepsilon(x, t - t'') dt'' \right]^2 \Big\} \\ &\quad \times \exp \left[ -k \int_0^{t'} [A^\varepsilon(x, t - t'')] dt'' \right] dt' \\ &\quad + k[1 - A^\varepsilon(x, t)] A^\varepsilon(x, t). \end{aligned} \quad (6)$$

We take into account that at finite times in the limit  $\varepsilon \rightarrow 0$  the exponent in the Eq. (6) tends to unity since  $A^\varepsilon(x, t'') \rightarrow 0$  exponentially fast due to Eq. (5). Namely,

$$\lim_{\varepsilon \rightarrow 0} \exp \left[ -k \int_0^{t'} [A^\varepsilon(x, t - t'')] dt'' \right] = 1.$$

Derivatives of  $A^\varepsilon(x, t)$  yield the following expressions

$$\partial_t A^\varepsilon = -(A_0/\varepsilon)(\partial_t G^\varepsilon) \exp(-G^\varepsilon/\varepsilon),$$

$$\Delta A^\varepsilon = \left[ (A_0/\varepsilon^2)(\partial_x G^\varepsilon)^2 - (A_0/\varepsilon)(\partial_x^2 G^\varepsilon) \right] \exp(-G^\varepsilon/\varepsilon).$$

We also take into account that the terms of the order of  $(A^\varepsilon(x, t))^2$  in braces tend to zero faster than  $\frac{\partial A^\varepsilon}{\partial t}$  and disappear in the limit  $\varepsilon \rightarrow 0$ . Keeping in mind this limit and substituting these expressions in Eq. (6), one obtains for  $G^\varepsilon \equiv G^\varepsilon(x, t)$

$$\begin{aligned} -\frac{\partial G^\varepsilon(x, t)}{\partial t} &= \sigma^2 \int_0^{t/\varepsilon} M(t') \left\{ \left[ \left( \frac{\partial G^\varepsilon}{\partial x} \right)^2 - \varepsilon \frac{\partial^2 G^\varepsilon}{\partial x^2} \right] \right. \\ &\quad \times \exp \left[ \frac{G^\varepsilon(x, t)}{\varepsilon} - \frac{G^\varepsilon(x, t - \varepsilon t')}{\varepsilon} \right] + k \left[ \left( \frac{\partial G^\varepsilon}{\partial x} \right)^2 - \varepsilon \frac{\partial^2 G^\varepsilon}{\partial x^2} \right] \\ &\quad \times \int_0^{t'} \exp \left[ \frac{G^\varepsilon(x, t)}{\varepsilon} - \frac{G^\varepsilon(x, t - t'')}{\varepsilon} \right] dt'' \Big\} dt' \\ &\quad + k[1 - A^\varepsilon(x, t)]. \end{aligned} \quad (7)$$

It follows from (5) that as long as the function

$$G(x, t) = \lim_{\varepsilon \rightarrow 0} G^\varepsilon(x, t) \quad (8)$$

is positive, the rescaled density  $A^\varepsilon(x, t) \rightarrow 0$  as  $\varepsilon \rightarrow 0$ . It also follows in this limit that  $\partial_x G(x, t - \varepsilon t') = \partial_x G(x, t)$  and

$$\lim_{\varepsilon \rightarrow 0} \left[ \frac{G^\varepsilon(x, t)}{\varepsilon} - \frac{G^\varepsilon(x, t - \varepsilon t')}{\varepsilon} \right] = [\partial_t G(x, t)] t'.$$

Taking into account this limit expression, we obtain the following equation for  $G(x, t)$

$$\begin{aligned} \frac{\partial G}{\partial t} &= -\sigma^2 \left( \frac{\partial G}{\partial x} \right)^2 \int_0^\infty M(t') \exp \left[ \frac{\partial G}{\partial t} t' \right] dt' \\ &\quad - k \sigma^2 \left( \frac{\partial G}{\partial x} \right)^2 \int_0^\infty M(t') \int_0^{t'} \exp \left[ \frac{\partial G}{\partial t} t'' \right] dt'' dt' - k. \end{aligned} \quad (9)$$

In what follows  $G(x, t)$  is the action, or Hamilton's principle function, such that

$$H = -\frac{\partial G}{\partial t}, \quad p = \frac{\partial G}{\partial x} \quad (10)$$

are the Hamiltonian, and the momentum, respectively. Therefore, it follows from Eq. (10) that Eq. (9) is a kind of Hamilton-Jacobi equation. The Laplace transform of the memory kernel yields

$$\tilde{M}(H) = \hat{\mathcal{L}} M(t) \int_0^\infty M(t') e^{-H t'} dt' = \frac{H \tilde{\psi}(H)}{1 - \tilde{\psi}(H)}, \quad (11)$$

where  $\tilde{\psi}(H) = \hat{\mathcal{L}}\psi(t)$  is the Laplace image of the waiting time pdf [see Eq. (2)]. Finally, one obtains that the Hamiltonian can be found from the Hamilton-Jacobi equation

$$\begin{aligned} \frac{\partial G}{\partial t} &= -\sigma^2 \left( \frac{\partial G}{\partial x} \right)^2 \tilde{M}(H) \\ &+ \frac{k\sigma^2}{H} \left( \frac{\partial G}{\partial x} \right)^2 [\tilde{M}(H) - \tilde{M}(0)] - k. \end{aligned} \quad (12)$$

Eventually, it reads

$$H = \sigma^2 p^2 \tilde{M}(H) - \frac{k\sigma^2}{H} p^2 [\tilde{M}(H) - \tilde{M}(0)] + k, \quad (13)$$

and the action is  $G(x, t) = \int_0^t [p(s)\dot{x}(s) - H(p(s), x(s))] ds$ .

The rate  $v$  at which the front moves is determined from Eq. (5) at the condition  $G(x, t) = 0$ . Together with the Hamilton equations, this yields

$$v = \dot{x} = \frac{\partial H}{\partial p}, \quad v = \frac{H}{p}. \quad (14)$$

Note that the first equation reflects the dispersion condition, while the second one is a result of the asymptotically free particle dynamics, when the action is  $G(x, t) = px - Ht$ . Taking into account  $x = vt$ , one obtains Eq. (14) (see also details of this discussion *e.g.* in Refs. [13, 18]). Now we analyze these two Eqs. (14) to define  $v$ .

*Markovian case.-*

First let us check the Markovian case, when  $\psi = \frac{1}{\tau} \exp(-t/\tau)$ . Thus one has

$$\tilde{\psi}(H) = \frac{1}{1 + H\tau},$$

where  $\tau$  is a characteristic time scale. Therefore, from Eq. (11) the Laplace image of the memory kernel reads

$$\tilde{M}(H) = \tilde{M}(0) = 1/\tau. \quad (15)$$

In this case, the Hamiltonian in Eq. (13) is  $H = Dp^2 + k$ , where  $\sigma^2/\tau = D$  is a diffusion coefficient. The moment is

$$p(H) = \sqrt{\frac{1}{D}(H - k)}.$$

From Eqs. (14) we have  $2Dp = H/p$  and  $H = 2k$ , which yields for the overall velocity of the front propagation

$$v = 2\sqrt{kD}, \quad (16)$$

which is the classical FKPP propagation speed (see discussions in Refs. [5, 19]).

*Subdiffusion.-* We have for subdiffusion  $\psi = \frac{1}{1+(t/\tau)^{1+\alpha}}$ , which yields [5, 19]

$$\tilde{M}(H) = \frac{H^{1-\alpha}}{\tau^\alpha}, \quad (\tilde{M}(0) = 0), \quad (17)$$

where the transport exponent is defined in the range  $0 < \alpha < 1$ . The Hamiltonian is

$$H = D_\alpha(H - k)H^{-\alpha}p^2 + k, \quad (18)$$

where  $D_\alpha = \sigma^2/\tau^\alpha$  is a generalized diffusion coefficient. From Eq. (18) one obtains

$$p(H) = \sqrt{\frac{H^\alpha}{D_\alpha}}, \quad (19)$$

and Eqs. (14) result in

$$\frac{\partial H}{\partial p} - \frac{H}{p} = 0 = \sqrt{D_\alpha} \left( \frac{2}{\alpha} - 1 \right) H^{1-\frac{\alpha}{2}}. \quad (20)$$

This equation has the solution for  $H = \tilde{H} = 0$ . Therefore, the asymptotic velocity of the front propagation is

$$v(\tilde{H}) = 0.$$

*Conclusion.-* We demonstrated the technique of hyperbolic scaling for the calculation of the reaction front velocity in an irreversible autocatalytic conversion reaction  $A + B \rightarrow 2A$  under subdiffusion. This is a technical presentation of the powerful Hamilton-Jacobi method for asymptotic estimation of the propagation front velocity observed in Ref. [5].

It should be admitted that the dispersion velocity  $v(H)$  also determines the relaxation rate at the large time asymptotic  $t \rightarrow \infty$  for the *finite* value of  $H$ . A qualitative crossover argument based on the truncated power-law distribution was suggested in Ref. [11]. According to the arguments, for short times the behavior of the velocity  $v(H)$  must be similar to that in subdiffusion (it does not feel the cutoff), whereas for long times the behavior is the classical one with a constant minimal velocity, and there has to be a crossover (no jump!) at a time  $t_{\text{cr}}$  between the two of them. Assuming that the time dependence of the velocity in the anomalous domain is  $v(t) \sim t^\beta$  and, after the crossover to the normal domain, the velocity, determined by Eq. (16),  $v = 2\sqrt{kD}$  is attained, both can be equated at  $t_{\text{cr}}$  to obtain the corresponding  $\beta$ . To determine the crossover time, it is plausible to argue with the amount of performed steps, as a measure of mobility, which for the normal regime is  $n_D(t) \propto t/t^{1-\alpha}T^\alpha$  and in the subdiffusive regime reads  $n_{SD}(t) \propto (t/t_0)^\alpha$ , equating them, one finds  $v(t < t_{\text{cr}}) \sim t^{\frac{1-\alpha}{2}}$ .

The hyperbolic scaling also corroborates the relaxation picture for the velocity  $v(H) \sim t^{\frac{\alpha-1}{2}}$  obtained in Refs. [10, 11]. An important point when considering the relaxation in the framework of hyperbolic scaling is that the process of relaxation for a subdiffusive front can be treated for the finite energy  $H = 2k$  in the framework of the Markovian case. For normal diffusion, the hyperbolic scaling method is rigorously justified [12], and the method yields a correct result for  $v(H)$  in Eq. (16), which is exactly the FKPP case. This can be demonstrated for

a truncated waiting time pdf  $\psi_T(t)$ . The latter is convenient to take, *e.g.*, in the following power-law form

$$\psi_T(t) = \frac{[1 + (t_0/T)^\alpha] e^{-t/T}}{1 + (t/t_0)^{\alpha+1}}, \quad (21)$$

where  $T$  has the role of the cutoff. Therefore, for any finite  $T$  the mean waiting time is finite:

$$\tau = \frac{\alpha t_0^\alpha}{1 + (t_0/T)^\alpha} T^{1-\alpha}.$$

For this normal diffusion hyperbolic scaling yields Eq. (16) for the velocity in the form

$$v(T) \propto \sqrt{Dk} \propto T^{\frac{\alpha-1}{2}}, \quad (22)$$

which corresponds to the relaxation rate obtained in Ref. [11].

Another specific property of the method is an effective linearization of the generalized FKPP Eq. (4). It should be admitted that this relates to considering a wavefront

with an exponentially decaying leading edge moving with a constant velocity  $v$ . The standard, traditional way to perform this analysis is first to linearize the equations. Hyperbolic scaling performs it automatically, since the density  $A$  is not zero only when  $G = 0$ . Moreover, it also affects the integrand kernel in Eq. (4), namely, as admitted above, in the limit  $\varepsilon \rightarrow 0$ , the exponent in the Eq. (6) tends to unity since  $A^\varepsilon(x, t'') \rightarrow 0$  exponentially fast due to Eq. (5). This essential simplification makes it possible to apply the strong machinery of the Laplace transform and arrive at the analytically treatable Hamilton-Jacobi equation (12) that is an easy and elegant way to obtain the front propagation, namely the failure of the latter. This nonlinear kernel was also studied in relation to a mechanism coupling the waiting time distributions to the reaction [7] to resolve a controversy about reaction-subdiffusion front propagation. To this end, a more general scheme of the local waiting time was suggested [7] that eventually leads to a more complicated analysis in the framework of the Hamilton-Jacobi approach than presented here.

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